Bis(2-ethylhexyl) phosphate 298-07-7 | DTXSID1027134

Model Performance

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.84	0.55	0.85	0.53	0.83	0.64	

Model Results

Predicted value: 5.58

Global applicability domain: Inside

Local applicability domain index: 2.16e-01

Confidence level: 6.51e-01

Nearest Neighbors from the Training Set

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Bis(2-ethylhexyl) phosphate

Measured: 4.37 **Predicted:** 5.58

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Docusate sodium Measured: 9.33 Predicted: 8.95

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2-Ethylhexyl diphenyl phosphate

Measured: 309 Predicted: 31.9

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Abietic acid Measured: 93.3 Predicted: 74.1

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Palustric acid
Measured: 25.1
Predicted: 41.8